W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:10 PM GMT

PDB ID	:	4XS4
Title	:	Salmonella typhimurium AhpC C165S mutant
Authors	:	Perkins, A.; Nelson, K.; Parsonage, D.; Poole, L.; Karplus, P.A.
Deposited on	:	2015-01-21
Resolution	:	2.65 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

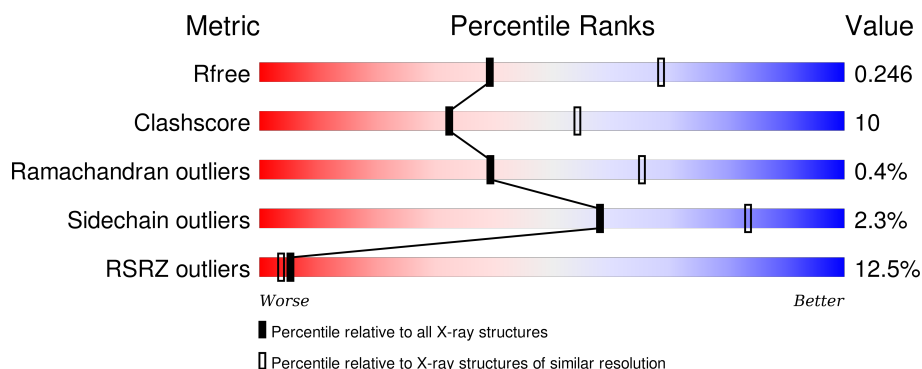|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.246
Clashscore		10
Ramachandran outliers		0.4%
Sidechain outliers		2.3%
RSRZ outliers		12.5%

Worse → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	186	2% / 74% · 15% · 10%
1	C	186	13% / 82% · 13% ·
1	D	186	13% / 83% · 15% ·
1	E	186	20% / 77% · 20% ·
2	B	186	13% / 82% · 13% · ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	K	A	201	-	-	-	X
3	K	D	201	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7688 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alkyl hydroperoxide reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	10	0
			1389	884	228	273	4			
1	C	186	Total	C	N	O	S	0	2	0
			1473	938	244	288	3			
1	D	186	Total	C	N	O	S	0	1	0
			1462	931	242	286	3			
1	E	186	Total	C	N	O	S	0	1	0
			1464	932	242	287	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	SER	CYS	engineered mutation	UNP P0A251
C	165	SER	CYS	engineered mutation	UNP P0A251
D	165	SER	CYS	engineered mutation	UNP P0A251
E	165	SER	CYS	engineered mutation	UNP P0A251

- Molecule 2 is a protein called Alkyl hydroperoxide reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	186	Total	C	N	O	S	0	9	0
			1531	976	254	297	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	165	SER	CYS	engineered mutation	UNP P0A251

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	K 1	0	0
3	A	1	Total 1	K 1	0	0
3	D	1	Total 1	K 1	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total 90	O 90	0	0
4	B	94	Total 94	O 94	0	0
4	C	79	Total 79	O 79	0	0
4	D	80	Total 80	O 80	0	0
4	E	23	Total 23	O 23	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
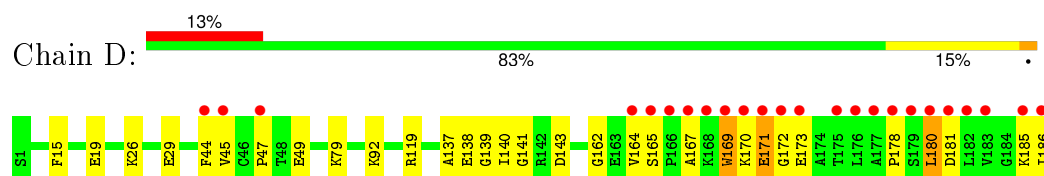
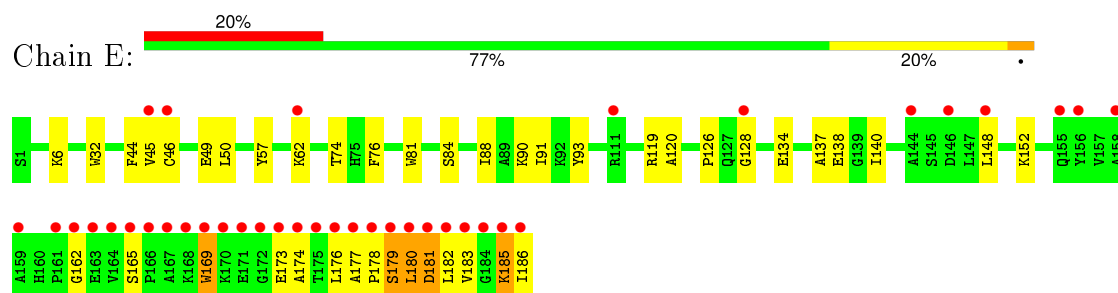• Molecule 1: Alkyl hydroperoxide reductase subunit C
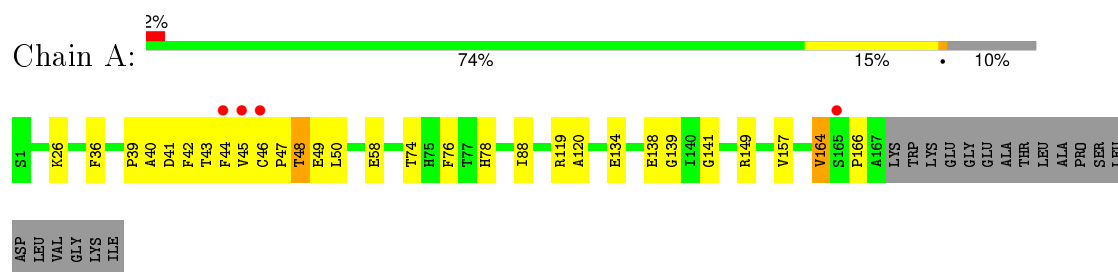
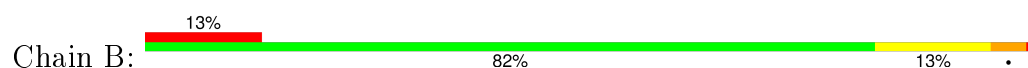• Molecule 1: Alkyl hydroperoxide reductase subunit C
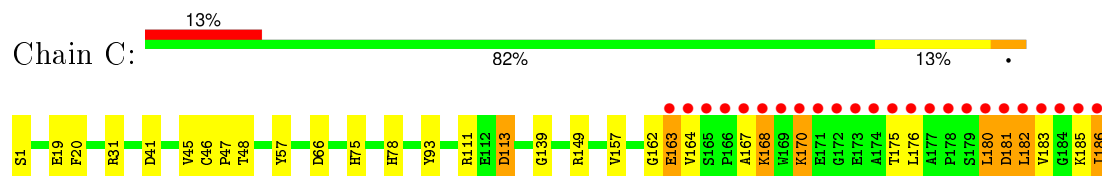
• Molecule 1: Alkyl hydroperoxide reductase subunit C

• Molecule 1: Alkyl hydroperoxide reductase subunit C

• Molecule 2: Alkyl hydroperoxide reductase subunit C

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	127.05Å 172.10Å 136.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.11 – 2.65 68.11 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.11-2.65) 100.0 (68.11-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.28 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.202 , 0.245 0.206 , 0.246	Depositor DCC
R_{free} test set	2160 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.51, <L^2> = 0.34$	Xtriage
Outliers	0 of 43635 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7688	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, OCS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.64	0/1423	0.86	3/1932 (0.2%)
1	C	0.68	0/1507	1.00	7/2041 (0.3%)
1	D	0.65	0/1496	0.86	2/2027 (0.1%)
1	E	0.62	2/1498 (0.1%)	0.97	4/2030 (0.2%)
2	B	0.72	1/1551 (0.1%)	1.11	11/2098 (0.5%)
All	All	0.66	3/7475 (0.0%)	0.97	27/10128 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	169	TRP	CB-CG	-5.75	1.39	1.50
1	E	173	GLU	CB-CG	5.40	1.62	1.52
2	B	183	VAL	CB-CG1	-5.07	1.42	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	176	LEU	CA-CB-CG	-12.62	86.27	115.30
2	B	183	VAL	CG1-CB-CG2	-11.99	91.71	110.90
2	B	182	LEU	N-CA-C	10.98	140.66	111.00
2	B	182	LEU	CB-CG-CD2	-10.46	93.22	111.00
2	B	182	LEU	N-CA-CB	-9.71	90.99	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	182	LEU	CA-CB-CG	9.69	137.59	115.30
1	C	186	ILE	CG1-CB-CG2	-8.42	92.88	111.40
1	C	181	ASP	N-CA-CB	-7.80	96.57	110.60
1	E	44	PHE	CB-CG-CD1	-7.51	115.54	120.80
2	B	183	VAL	C-N-CA	7.47	137.99	122.30
2	B	177	ALA	N-CA-C	7.41	131.00	111.00
1	C	180	LEU	CA-CB-CG	7.01	131.42	115.30
2	B	182	LEU	C-N-CA	-6.97	104.29	121.70
1	E	180	LEU	CA-CB-CG	6.45	130.13	115.30
1	A	149	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	D	169	TRP	C-N-CA	5.80	136.19	121.70
1	C	168	LYS	CD-CE-NZ	5.78	124.98	111.70
1	C	163	GLU	CB-CA-C	-5.72	98.97	110.40
1	E	44	PHE	CB-CG-CD2	5.67	124.77	120.80
1	A	26	LYS	CB-CG-CD	5.66	126.31	111.60
1	C	182	LEU	CA-CB-CG	5.62	128.22	115.30
1	C	168	LYS	N-CA-CB	5.43	120.37	110.60
1	E	174	ALA	N-CA-C	5.40	125.58	111.00
2	B	176	LEU	CB-CG-CD1	5.37	120.13	111.00
2	B	182	LEU	CA-C-N	5.22	128.69	117.20
1	D	172	GLY	N-CA-C	5.17	126.03	113.10
1	A	26	LYS	CA-CB-CG	-5.00	102.40	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	181	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1389	0	1327	35	0
1	C	1473	0	1433	34	0
1	D	1462	0	1422	37	0
1	E	1464	0	1421	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1531	0	1483	51	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	90	0	0	2	0
4	B	94	0	0	0	1
4	C	79	0	0	1	0
4	D	80	0	0	0	1
4	E	23	0	0	0	0
All	All	7688	0	7086	151	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ALA:O	2:B:168:LYS:HB3	1.63	0.96
2:B:183:VAL:HG12	2:B:184:GLY:N	1.75	0.95
1:A:49:GLU:HG2	2:B:167:ALA:HB2	1.48	0.94
2:B:183:VAL:HG12	2:B:184:GLY:H	1.29	0.93
1:C:45:VAL:HG22	1:D:164:VAL:HG11	1.53	0.90
1:E:182:LEU:HG	1:E:185:LYS:HD3	1.56	0.86
1:A:42[B]:PHE:O	2:B:183:VAL:HG11	1.75	0.85
2:B:183:VAL:CG1	2:B:184:GLY:H	1.88	0.84
1:A:46[A]:CYS:HA	2:B:186:ILE:HG21	1.59	0.84
1:C:163:GLU:N	1:C:163:GLU:OE1	2.11	0.83
1:D:165:SER:HB3	1:D:169:TRP:CG	2.15	0.82
1:A:44[A]:PHE:CD1	2:B:182:LEU:HD21	2.17	0.79
1:C:45:VAL:CG2	1:D:164:VAL:HG11	2.12	0.78
1:D:170:LYS:N	1:D:173:GLU:OE2	2.15	0.78
2:B:182:LEU:HG	2:B:183:VAL:HG23	1.66	0.77
1:E:119:ARG:NH2	1:E:138:GLU:OE2	2.16	0.76
1:A:42[B]:PHE:C	2:B:183:VAL:HG11	2.09	0.73
1:A:44[A]:PHE:CE1	2:B:182:LEU:HD21	2.25	0.72
1:C:167:ALA:HB2	1:D:49:GLU:HG2	1.71	0.71
1:E:182:LEU:HD21	1:E:186:ILE:HG12	1.72	0.71
1:C:176:LEU:HD21	1:C:186:ILE:HD12	1.72	0.69
1:E:165:SER:HB3	1:E:169:TRP:NE1	2.07	0.69
2:B:162:GLY:O	2:B:178:PRO:HD2	1.92	0.69
1:E:182:LEU:HD23	1:E:182:LEU:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:SER:HB2	2:B:182:LEU:HD13	1.74	0.67
1:C:183:VAL:HA	1:D:44:PHE:CE1	2.30	0.67
1:E:137:ALA:HB3	1:E:140:ILE:HD12	1.76	0.67
1:D:162:GLY:O	1:D:178:PRO:HD2	1.95	0.66
1:E:182:LEU:HD21	1:E:186:ILE:HG23	1.77	0.66
2:B:79:LYS:NZ	1:D:180:LEU:O	2.28	0.66
1:A:139:GLY:HA3	2:B:157:VAL:HG11	1.76	0.66
1:E:62:LYS:O	1:E:62:LYS:HD2	1.95	0.65
1:E:45:VAL:HG11	1:E:119:ARG:NH2	2.12	0.65
2:B:45[B]:VAL:HG11	2:B:138:GLU:OE1	1.97	0.64
2:B:168:LYS:HE3	2:B:173:GLU:OE2	1.99	0.62
1:C:183:VAL:HA	1:D:44:PHE:CZ	2.34	0.62
1:C:182:LEU:HG	1:D:44:PHE:CE1	2.34	0.62
1:E:50:LEU:HB3	1:E:91:ILE:HD11	1.82	0.61
1:E:6:LYS:NZ	1:E:128:GLY:HA3	2.16	0.60
2:B:169:TRP:HZ3	2:B:173:GLU:O	1.85	0.60
1:A:40:ALA:O	1:A:43[B]:THR:OG1	2.10	0.60
2:B:15:PHE:CE1	2:B:79:LYS:HG3	2.36	0.60
2:B:176:LEU:HD23	2:B:177:ALA:H	1.68	0.59
1:C:182:LEU:HA	1:C:185:LYS:HD3	1.84	0.59
1:D:26:LYS:HA	1:D:29:GLU:HG3	1.83	0.59
1:A:45[B]:VAL:HG13	2:B:166:PRO:HA	1.84	0.59
1:D:119:ARG:NH2	1:D:138:GLU:OE1	2.36	0.59
1:C:139:GLY:HA2	1:D:164:VAL:HG22	1.84	0.59
1:E:182:LEU:O	1:E:185:LYS:HB3	2.01	0.58
1:C:164:VAL:HG11	1:D:45:VAL:HG21	1.86	0.58
1:A:44[B]:PHE:C	1:A:47[B]:PRO:HD2	2.23	0.58
1:A:44[B]:PHE:O	1:A:47[B]:PRO:HD2	2.04	0.57
2:B:182:LEU:CG	2:B:183:VAL:HG23	2.33	0.57
1:D:137:ALA:HB3	1:D:140:ILE:HD12	1.86	0.57
1:E:165:SER:HB3	1:E:169:TRP:CD1	2.39	0.57
1:E:181:ASP:HA	1:E:183:VAL:H	1.70	0.57
1:A:42[A]:PHE:C	2:B:183:VAL:HG11	2.24	0.56
1:A:39:PRO:HD2	1:A:46[B]:CYS:SG	2.45	0.56
1:C:182:LEU:HG	1:D:44:PHE:CD1	2.40	0.56
2:B:177:ALA:O	2:B:178:PRO:C	2.44	0.55
1:C:48:THR:HG22	1:D:167:ALA:HB3	1.88	0.55
1:A:164:VAL:HG11	2:B:45[B]:VAL:HG22	1.88	0.55
1:C:168:LYS:HE2	1:D:143:ASP:OD2	2.07	0.55
1:E:182:LEU:CD2	1:E:186:ILE:HG12	2.37	0.54
1:E:6:LYS:HZ3	1:E:128:GLY:HA3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:CYS:N	1:C:47:PRO:HD2	2.23	0.54
1:A:47[B]:PRO:HB3	1:A:88:ILE:HD11	1.89	0.54
1:A:157:VAL:HG11	2:B:139:GLY:HA3	1.90	0.54
1:A:47[B]:PRO:HA	1:A:50:LEU:HD12	1.90	0.53
1:A:139:GLY:O	2:B:165:SER:HB2	2.09	0.53
2:B:177:ALA:O	2:B:179:SER:OG	2.28	0.52
1:E:57:TYR:CE1	1:E:93:TYR:HB3	2.43	0.52
1:A:46[A]:CYS:HB2	2:B:176:LEU:CD1	2.39	0.52
1:E:178:PRO:O	1:E:179:SER:OG	2.25	0.52
2:B:179:SER:CB	2:B:182:LEU:HD13	2.39	0.52
1:E:181:ASP:HA	1:E:183:VAL:HG22	1.91	0.52
1:C:31:ARG:HD3	1:C:66:ASP:OD2	2.10	0.51
2:B:163:GLU:OE1	2:B:175:THR:HG21	2.11	0.50
1:D:164:VAL:HG13	1:D:165:SER:N	2.27	0.50
1:D:181:ASP:O	1:D:185:LYS:HE2	2.11	0.50
1:A:36:PHE:HZ	1:A:49:GLU:HB3	1.76	0.50
1:E:183:VAL:O	1:E:183:VAL:HG23	2.12	0.50
1:C:47:PRO:HG3	1:D:186:ILE:CG2	2.42	0.50
1:E:32:TRP:CE2	1:E:126:PRO:HD3	2.47	0.50
1:D:170:LYS:CG	1:D:171:GLU:N	2.75	0.49
1:C:180:LEU:HD12	1:C:181:ASP:N	2.27	0.49
1:A:74:THR:OG1	1:A:76:PHE:HB2	2.11	0.49
1:E:46:CYS:O	1:E:49:GLU:HB2	2.12	0.49
1:E:120:ALA:HA	1:E:134:GLU:O	2.12	0.49
1:E:148:LEU:O	1:E:152:LYS:HG2	2.12	0.49
1:D:170:LYS:HG2	1:D:171:GLU:N	2.28	0.49
1:C:176:LEU:HD21	1:C:186:ILE:CD1	2.43	0.49
1:E:165:SER:HB3	1:E:169:TRP:HE1	1.77	0.49
2:B:182:LEU:HG	2:B:183:VAL:CG2	2.40	0.48
1:D:15:PHE:CE1	1:D:79:LYS:HG3	2.48	0.48
2:B:169:TRP:CZ3	2:B:173:GLU:O	2.64	0.48
1:A:119:ARG:HE	1:A:138:GLU:HA	1.78	0.48
1:D:19:GLU:OE1	1:D:19:GLU:HA	2.14	0.47
1:C:41:ASP:OD2	1:C:78:HIS:ND1	2.45	0.47
1:D:44:PHE:C	1:D:47:PRO:HD2	2.35	0.47
1:A:44[A]:PHE:HA	2:B:182:LEU:HG	1.96	0.47
1:A:43[A]:THR:C	2:B:183:VAL:HG21	2.36	0.46
1:E:182:LEU:HD21	1:E:186:ILE:CG1	2.44	0.46
1:C:183:VAL:CG2	1:D:44:PHE:HZ	2.29	0.46
1:C:111:ARG:HB3	1:C:113[A]:ASP:OD2	2.16	0.45
1:E:74:THR:OG1	1:E:76:PHE:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:HB2	4:A:349:HOH:O	2.16	0.45
1:E:176:LEU:HD23	1:E:177:ALA:N	2.32	0.45
1:E:81:TRP:CE2	1:E:88:ILE:HG13	2.51	0.45
1:A:120:ALA:HA	1:A:134:GLU:O	2.17	0.45
2:B:109:ASN:OD1	2:B:118:ASP:HB2	2.17	0.45
1:C:183:VAL:HG22	1:D:44:PHE:HZ	1.80	0.45
1:E:177:ALA:HA	1:E:178:PRO:HD2	1.69	0.45
1:A:46[A]:CYS:O	1:A:48[A]:THR:N	2.48	0.45
2:B:179:SER:C	2:B:182:LEU:HD22	2.37	0.45
1:C:149:ARG:NH2	1:D:141:GLY:O	2.37	0.45
1:C:183:VAL:HA	1:D:44:PHE:HE1	1.79	0.44
2:B:16:LYS:O	2:B:19:GLU:HG3	2.17	0.44
2:B:176:LEU:CD2	2:B:177:ALA:H	2.30	0.44
1:A:44[B]:PHE:CE1	2:B:182:LEU:HD11	2.53	0.44
2:B:168:LYS:HE3	2:B:173:GLU:CD	2.38	0.44
1:E:182:LEU:CG	1:E:185:LYS:HD3	2.40	0.44
2:B:175:THR:HG23	2:B:176:LEU:N	2.33	0.43
2:B:162:GLY:O	2:B:178:PRO:CD	2.63	0.43
1:A:47[A]:PRO:HD2	2:B:186:ILE:HG22	2.01	0.43
2:B:183:VAL:CG1	2:B:184:GLY:N	2.48	0.43
1:C:162:GLY:N	1:C:163:GLU:OE1	2.52	0.43
1:D:169:TRP:HA	1:D:173:GLU:OE2	2.18	0.43
1:C:164:VAL:HG13	1:D:139:GLY:HA2	2.01	0.43
1:C:57:TYR:CE1	1:C:93:TYR:HB3	2.54	0.43
1:A:141:GLY:O	2:B:149:ARG:NH2	2.29	0.42
1:C:139:GLY:N	4:C:230:HOH:O	2.34	0.42
1:E:119:ARG:HE	1:E:138:GLU:HA	1.84	0.42
2:B:185:LYS:HA	2:B:185:LYS:HD2	1.55	0.42
1:A:139:GLY:N	4:A:338:HOH:O	2.38	0.42
1:C:168:LYS:O	1:C:170:LYS:HE2	2.19	0.42
1:D:92:LYS:HE2	1:D:92:LYS:HB3	1.86	0.42
1:C:20:PHE:CD1	1:C:75:HIS:HD2	2.38	0.42
1:D:170:LYS:H	1:D:173:GLU:CD	2.13	0.41
1:C:181:ASP:OD1	1:C:181:ASP:C	2.59	0.41
1:A:166:PRO:O	2:B:46[A]:OCS:HB3	2.20	0.41
1:A:45[B]:VAL:CG2	2:B:164:VAL:HG21	2.51	0.41
1:C:157:VAL:HG11	1:D:139:GLY:HA3	2.03	0.41
1:E:162:GLY:O	1:E:178:PRO:HD2	2.21	0.41
1:A:41:ASP:OD2	1:A:78:HIS:ND1	2.39	0.41
1:A:40:ALA:HB3	1:A:43[A]:THR:HG21	2.03	0.40
1:C:164:VAL:CG1	1:D:139:GLY:HA2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LEU:HA	2:B:176:LEU:HD23	1.37	0.40
1:D:169:TRP:HA	1:D:173:GLU:OE1	2.22	0.40
1:E:45:VAL:HG13	1:E:46:CYS:N	2.37	0.40
2:B:32:TRP:CE2	2:B:126:PRO:HD3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:307:HOH:O	4:D:302:HOH:O[8_457]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	175/186 (94%)	168 (96%)	7 (4%)	0	100	100
1	C	186/186 (100%)	181 (97%)	5 (3%)	0	100	100
1	D	185/186 (100%)	181 (98%)	4 (2%)	0	100	100
1	E	185/186 (100%)	178 (96%)	5 (3%)	2 (1%)	17	38
2	B	191/186 (103%)	188 (98%)	1 (0%)	2 (1%)	19	41
All	All	922/930 (99%)	896 (97%)	22 (2%)	4 (0%)	39	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	179	SER
1	E	180	LEU
2	B	168	LYS
2	B	178	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	149/154 (97%)	146 (98%)	3 (2%)	63	86
1	C	156/154 (101%)	150 (96%)	6 (4%)	40	68
1	D	155/154 (101%)	153 (99%)	2 (1%)	76	91
1	E	155/154 (101%)	152 (98%)	3 (2%)	65	87
2	B	160/153 (105%)	155 (97%)	5 (3%)	47	75
All	All	775/769 (101%)	756 (98%)	19 (2%)	58	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48[A]	THR
1	A	48[B]	THR
1	A	164	VAL
2	B	86	GLU
2	B	164	VAL
2	B	175	THR
2	B	179	SER
2	B	182	LEU
1	C	1	SER
1	C	19	GLU
1	C	113[A]	ASP
1	C	113[B]	ASP
1	C	170	LYS
1	C	175	THR
1	D	171	GLU
1	D	180	LEU
1	E	84	SER
1	E	90	LYS
1	E	185	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	OCS	B	46[A]	2	6,8,9	2.12	1 (16%)	7,11,13	2.62	3 (42%)
2	OCS	B	46[B]	2	3,5,9	0.83	0	3,5,13	1.54	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OCS	B	46[A]	2	-	1/4/7/9	0/0/0/0
2	OCS	B	46[B]	2	-	0/1/4/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	46[A]	OCS	CB-SG	4.80	1.83	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	46[B]	OCS	O-C-CA	-2.62	118.69	125.72
2	B	46[A]	OCS	O-C-CA	-2.03	120.27	125.72
2	B	46[A]	OCS	OD1-SG-CB	4.08	109.80	106.92
2	B	46[A]	OCS	OD3-SG-CB	4.37	110.00	106.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	46[A]	OCS	SG-CB-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	46[A]	OCS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	167/186 (89%)	0.02	4 (2%)	62	60	24, 42, 85, 153	0
1	C	186/186 (100%)	0.58	24 (12%)	5	3	26, 52, 151, 199	22 (11%)
1	D	186/186 (100%)	0.62	24 (12%)	5	3	33, 52, 139, 157	22 (11%)
1	E	186/186 (100%)	1.14	38 (20%)	1	1	47, 80, 170, 189	22 (11%)
2	B	185/186 (99%)	0.58	24 (12%)	5	3	21, 40, 111, 160	23 (12%)
All	All	910/930 (97%)	0.60	114 (12%)	5	4	21, 52, 146, 199	89 (9%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	169	TRP	12.5
1	E	175	THR	10.1
1	C	170	LYS	9.9
2	B	183	VAL	9.1
2	B	169	TRP	9.0
1	D	167	ALA	8.6
2	B	180	LEU	8.2
2	B	182	LEU	8.2
1	C	172	GLY	8.0
2	B	179	SER	7.8
1	E	174	ALA	7.7
1	E	172	GLY	7.7
1	C	182	LEU	7.7
1	C	171	GLU	7.6
2	B	178	PRO	7.5
2	B	181	ASP	7.4
1	E	169	TRP	7.4
1	D	176	LEU	7.3
1	C	180	LEU	7.1
1	E	183	VAL	7.0

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Mol	Chain	Res	Type	RSRZ
1	D	165	SER	7.0
2	B	171	GLU	6.7
1	D	172	GLY	6.6
1	E	171	GLU	6.6
1	E	167	ALA	6.5
1	C	165	SER	6.4
1	D	180	LEU	6.3
2	B	168	LYS	6.2
1	E	176	LEU	6.2
1	E	182	LEU	6.2
1	D	166	PRO	6.1
1	D	178	PRO	6.1
2	B	174	ALA	6.0
2	B	185	LYS	5.9
1	E	164	VAL	5.8
2	B	167	ALA	5.8
1	D	183	VAL	5.7
1	C	174	ALA	5.7
1	D	164	VAL	5.7
1	D	185	LYS	5.6
1	D	179	SER	5.6
2	B	177	ALA	5.5
2	B	170	LYS	5.4
1	C	169	TRP	5.4
1	D	177	ALA	5.4
1	E	166	PRO	5.3
2	B	184	GLY	5.2
1	E	165	SER	5.2
1	E	170	LYS	5.1
1	D	173	GLU	5.1
1	E	159	ALA	5.1
1	D	175	THR	5.0
1	C	167	ALA	4.9
1	E	46	CYS	4.8
1	C	166	PRO	4.7
1	C	177	ALA	4.7
1	D	186	ILE	4.7
1	E	185	LYS	4.5
1	D	171	GLU	4.5
1	C	164	VAL	4.5
2	B	175	THR	4.4
1	E	168	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	184	GLY	4.3
1	D	170	LYS	4.2
1	A	44[A]	PHE	4.2
1	E	177	ALA	4.1
1	C	184	GLY	4.1
1	A	165	SER	4.1
1	E	178	PRO	4.1
1	C	185	LYS	4.0
1	E	186	ILE	4.0
2	B	172	GLY	3.7
1	D	181	ASP	3.6
2	B	164	VAL	3.5
1	C	178	PRO	3.5
1	C	186	ILE	3.5
1	E	180	LEU	3.4
1	E	161	PRO	3.4
1	D	182	LEU	3.4
1	E	163	GLU	3.2
1	C	183	VAL	3.2
1	E	156	TYR	3.2
1	C	181	ASP	3.1
1	D	168	LYS	3.1
1	A	46[A]	CYS	3.1
2	B	176	LEU	3.0
1	E	45	VAL	3.0
1	E	62	LYS	3.0
2	B	173	GLU	3.0
1	D	47	PRO	2.8
2	B	186	ILE	2.8
1	E	173	GLU	2.8
1	E	128	GLY	2.8
1	C	176	LEU	2.8
1	E	162	GLY	2.8
1	C	175	THR	2.8
1	E	144	ALA	2.5
1	E	148	LEU	2.5
1	A	45[A]	VAL	2.5
1	C	168	LYS	2.4
2	B	163	GLU	2.4
1	D	44	PHE	2.4
1	C	163	GLU	2.4
1	C	179	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	179	SER	2.4
1	E	158	ALA	2.3
2	B	166	PRO	2.3
2	B	165	SER	2.3
1	C	173	GLU	2.2
1	E	155	GLN	2.2
1	D	45	VAL	2.2
1	E	146[A]	ASP	2.1
1	E	181	ASP	2.1
1	E	111	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	OCS	B	46[B]	6/10	0.78	0.34	-	24,31,34,35	6
2	OCS	B	46[A]	9/10	0.78	0.34	-	41,49,79,79	9

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	K	A	201	1/1	0.80	0.31	9.16	52,52,52,52	1
3	K	D	201	1/1	0.80	0.24	3.89	105,105,105,105	0
3	K	B	201	1/1	0.94	0.10	-3.62	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.